

Alanine, 2-methyl-  
62-57-7 | DTXSID0058772

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.67 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.67e-01

Confidence level: 7.89e-01

Nearest Neighbors from the Training Set

Image not found

Alanine, 2-methyl-

Measured: 1.76

Predicted: 1.67

Image not found

DL-alanine

Measured: 1.86

Predicted: 1.82